Useful Procedure for Computing the Lattice Green's Function for the Several Lattices (科学計算基本ライブラリーのアルゴリズム)

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1. Square Lattice with the Nearest and the Next Nearest Neighbor Interactions

We first consider the square lattice with the nearest and the next nearest neighbor interactions. The lattice Green's function $G(t;m,n;\gamma,2\beta)$ for this case is defined as the solution of the difference equation with the δ-function type inhomogeneous part:

$$
\begin{aligned}
&2t\,G(t;m,n;\gamma,2\beta)-\gamma\{G(t;m+1,n;\gamma,2\beta)+G(t;m-1,n;\gamma,2\beta)\\
&+G(t;m,n+1;\gamma,2\beta)+G(t;m,n-1;\gamma,2\beta)\}-\beta\{G(t;m+1,n+1;\gamma,2\beta)\\
&+G(t;m+1,n-1;\gamma,2\beta)+G(t;m-1,n+1;\gamma,2\beta)+G(t;m-1,n-1;\gamma,2\beta)\}\\
&=2\delta_{m,0}\,\delta_{n,0}\;. \qquad (1.1)
\end{aligned}
$$

The boundary value is zero at $m^2+n^2\to\infty$. The solution is given by

$$G(t;m,n;\gamma,2\beta)=\frac{1}{\pi^2}\int_0^{\pi}dy\int_0^{\pi}dz\,\frac{\cos my\,\cos nz}{t-\gamma\cos y-\gamma\cos z-2\beta\cos y\cos z}\;. \qquad (1.2)$$

From the several symmetry properties which are satisfied by (1.2), we restrict ourselves in the following to the case:

$$m\geq 0,\quad n\geq 0,\quad \gamma\geq 0,\quad \beta\geq 0$$

without loss of generality.

If $n=0$, the integration of (1.2) over z gives

$$G(t;m,0;\gamma,2\beta)=\frac{1}{\pi}\int_0^{\pi}dy\,\frac{\cos my}{\sqrt{(t-\gamma\cos y)^2-(\gamma+2\beta\cos y)^2}}. \tag{1.3}$$

When t is real and larger than $2\gamma+2\beta$, $G(t;m,n;\gamma,2\beta)$ is real. We first investigate this case and give a useful procedure of calculating $G(t;m,n;\gamma,2\beta)$. Then the expressions occured are analytically continued, so that the obtained procedure becomes useful also for the cases of an arbitrary complex value of t and $t<2\gamma+2\beta$.

The lattice Green's function $G(t;m,0;\gamma,2\beta)$ given by (1.3) is expressed as follows:

$$G(t;m,0;\gamma,2\beta)=\frac{1}{\pi\sqrt{\pm(\gamma^2-4\beta^2)}}\int_0^{\pi}dy\,\frac{\cos my}{\sqrt{\pm(\xi-\cos y)(\eta-\cos y)}} \tag{1.4}$$

where

$$\xi=\frac{t-\gamma}{\gamma+2\beta}\quad,\quad \eta=\frac{t+\gamma}{\gamma-2\beta} \tag{1.5}$$

When $2\beta>\gamma>0$, $\xi>1>-1>\eta$ and the negative sign in the square root must be used in (1.5), whereas, if $0<2\beta<\gamma$, $\eta>\xi>1>-1$ and the positive sign is used. We can easily show that $G(t;m,0;\gamma,2\beta)$ satisfies the following recurrence formula;

$$G(t;m+2,0)=\frac{1}{\gamma^2-4\beta^2}\Big\{2\gamma(t+2\beta)\Big[\frac{2m+1}{m+1}G(t;m+1,0)$$

$$+\frac{2m-1}{m+1}G(t;m-1,0)\Big]-\frac{2m}{m+1}(2t^2-\gamma^2-4\beta^2)\,G(t;m,0)$$

$$-\frac{m-1}{m+1}G(t;m-2,0)\Big\}. \tag{1.6}$$

Now the parameters γ and β in $G(t;m,0;\gamma,2\beta)$ are not written explicitly for brevity. This recurrence formula shows that one can calculate all the values along the axis from the knowledge of $G(t;m,0;\gamma,2\beta)$ for m=0,1 and 2.

For both cases $2\beta>\gamma>0$ and $\gamma>2\beta>0$, $G(t;m,0;\gamma,2\beta)$ for m=0,1 and 2 are as follows:

$$G(t;0,0;\gamma,2\beta)=\frac{2}{\pi(t+2\beta)}K(k) \qquad (1.7)$$

$$G(t;1,0;\gamma,2\beta)=\frac{2}{\pi(t+2\beta)}[\eta K(k)-(1+\eta)\Pi(\alpha^2;k)] \qquad (1.8)$$

$$G(t;2,0;\gamma,2\beta)=\frac{2}{\pi(t+2\beta)}[\eta K(k)+(\eta-1)(\xi+1)E(k)$$
$$-(\eta+\xi)(\eta+1)\Pi(\alpha^2;k)] \qquad (1.9)$$

where

$$k=\frac{2(2\beta t+\gamma^2)^{1/2}}{t+2\beta} \qquad (1.10)$$

$$\alpha^2=\frac{-2\gamma+4\beta}{t+2\beta}. \qquad (1.11)$$

Now one can calculate $G(t;m,0;\gamma,2\beta)$ for an arbitrary m with the aid of the recurrence formula (1.6) by starting with (1.7), (1.8) and (1.9) for both cases $2\beta>\gamma>0$ and $\gamma>2\beta>0$. In order to obtain the value

$G(t;m,n;\gamma,2\beta)$ at an arbitrary site (m,n), the difference equation (1.1) is used.

When t is a complex value, we have only to use the complete elliptic integrals with the complex modulus in (1.7), (1.8) and (1.9). If $t=s-i\varepsilon$ where ε is an infinitesimal positive number and $s<2\gamma+2\beta$, one uses the following analytic continuations:

$$K(k)=\frac{1}{k}\left[K\left(\frac{1}{k}\right)+iK\left(\frac{\sqrt{k^2-1}}{k}\right)\right] \tag{1.12}$$

$$E(k)=k\left[E\left(\frac{1}{k}\right)-\frac{k^2-1}{k^2}K\left(\frac{1}{k}\right)\right]-ik\left[E\left(\frac{\sqrt{k^2-1}}{k}\right)-\frac{1}{k^2}K\left(\frac{\sqrt{k^2-1}}{k}\right)\right] \tag{1.13}$$

$$\Pi(\alpha^2,k)=\frac{1}{k}\Pi\left(\frac{\alpha^2}{k^2},\frac{1}{k}\right) \tag{1.14}$$

$$+i\frac{1}{k}\left[K\left(\frac{\sqrt{k^2-1}}{k}\right)+\frac{\alpha^2}{k^2-\alpha^2}\Pi\left(\frac{k^2-1}{k^2-\alpha^2},\frac{\sqrt{k^2-1}}{k}\right)\right] \tag{1.15}$$

for $k>1$, and their complex conjugate for $k<-1$,

$$\overset{(\mathrm{II})}{K}(k)=K(k)+2iK(k') \tag{1.16}$$

$$\overset{(\mathrm{II})}{E}(k)=E(k)+2i\left[K(k')-E(k')\right] \tag{1.17}$$

$$\overset{(\mathrm{II})}{\Pi}(\alpha^2,k)=\Pi(\alpha^2,k)+2i\left[K(k')+\frac{\alpha^2}{1-\alpha^2}\Pi\left(\frac{k'^2}{1-\alpha^2},k'\right)\right] \tag{1.18}$$

for $0<k<1$ on the sheet (II) which is reached through the branch cut connecting +1 and $+\infty$ by encircling around the poin $k=1$ anticlockwise,

$$K(ik_I)=\frac{1}{\sqrt{1+k_I^2}}K\left(\frac{k_I}{\sqrt{1+k_I^2}}\right) \tag{1.19}$$

$$E(ik_I)=\sqrt{1+k_I^2}\;E\left(\frac{k_I}{\sqrt{1+k_I^2}}\right) \tag{1.20}$$

$$\Pi(\alpha^2,ik_I)=\frac{1}{\sqrt{1+k_I^2}}\left[\frac{k_I^2}{\alpha^2+k_I^2}K\left(\frac{k_I}{\sqrt{1+k_I^2}}\right)+\frac{\alpha^2}{\alpha^2+k_I^2}\Pi\left(\frac{\alpha^2+k_I^2}{1+k_I^2},\frac{k_I}{\sqrt{1+k_I^2}}\right)\right] \tag{1.21}$$

for k which on the positive imaginary axis, $k=ik_I$, and

$$\overset{(\mathrm{II})}{K}(-ik_I+\varepsilon) = -\frac{1}{\sqrt{1+k_I^2}}\left[K\left(\frac{k_I}{\sqrt{1+k_I^2}}\right)+2iK\left(\frac{1}{\sqrt{1+k_I^2}}\right)\right] \tag{1.22}$$

$$\overset{(\mathrm{II})}{E}(-ik_I+\varepsilon) = 3\sqrt{1+k_I^2}\,E\left(\frac{k_I}{\sqrt{1+k_I^2}}\right)-\frac{4}{\sqrt{1+k_I^2}}K\left(\frac{k_I}{\sqrt{1+k_I^2}}\right)$$

$$+2i\left[\sqrt{1+k_I^2}\,E\left(\frac{1}{\sqrt{1+k_I^2}}\right)-\sqrt{1+k_I^2}\,K\left(\frac{1}{\sqrt{1+k_I^2}}\right)\right] \tag{1.23}$$

$$\overset{(\mathrm{II})}{\Pi}(-ik_I+\varepsilon) = \frac{1}{\sqrt{1+k_I^2}}\left[\frac{k_I^2\alpha^2+k_I^2+2\alpha^2}{(\alpha^2+k_I^2)(\alpha^2-1)}K\left(\frac{k_I}{\sqrt{1+k_I^2}}\right)+\frac{2}{1-\alpha^2}\Pi\left(\frac{\alpha^2-1}{\alpha^2(1+k_I^2)},\frac{k_I}{\sqrt{1+k_I^2}}\right)\right]$$

$$+2i\frac{1}{\sqrt{1+k_I^2}}\left[K\left(\frac{1}{\sqrt{1+k_I^2}}\right)+\frac{\alpha^2}{1-\alpha^2}\Pi\left(\frac{1}{1-\alpha^2},\frac{1}{\sqrt{1+k_I^2}}\right)\right] \tag{1.24}$$

for k which is on the negative imaginary axis on the sheet (II).

For all the ranges of s, we have the following cases and the ranges of k which correspond to each case,

(I) $2\beta > \gamma > 0$

$$\begin{array}{ll}
2\beta+2\gamma < s < \infty & 0 < k < 1 \\
2\beta-2\gamma < s < 2\beta+2\gamma & 1 < k < \infty \\
-\gamma^2/2\beta < s < 2\beta-2\gamma & 0 < k < 1 \quad (\mathrm{II}) \\
-2\beta < s < -\gamma^2/2\beta & k = -ik_I \quad (\mathrm{II}) \\
-\infty < s < -2\beta & k = ik_I
\end{array}$$

(II) $\gamma > 2\beta > 0$

$$\begin{array}{ll}
2\beta+2\gamma < s < \infty & 0 < k < 1 \\
-2\beta < s < 2\beta+2\gamma & 1 < k < \infty \\
2\beta-2\gamma < s < -2\beta & -\infty < k < -1 \\
-\gamma^2/2\beta < s < 2\beta-2\gamma & -1 < k < 0 \\
-\infty < s < -\gamma^2/2\beta & k = ik_I
\end{array}$$

where

$$k_I = \frac{2\sqrt{-2\beta s-\gamma^2}}{s+2\beta} \tag{1.25}$$

In each case, the corresponding expressions for $G(t;0,0;\gamma,2\beta)$, $G(t;1,0;\gamma,2\beta)$ and $G(t;2,0;\gamma,2\beta)$ are obtained from (1.7), (1.8) and (1.9) using (1.12)-(1.24).

Now we can obtain the value $G(s-i\varepsilon,m,n;\gamma,2\beta)$ at an arbitrary lattice point for all the ranges of s from (1.6)and (1.1).

2. S.C. and Tetragonal Lattices

The lattice Green's function for the tetragonal lattice is given by

$$G(t;l,m,n)=\frac{1}{\pi^3}\int_0^\pi dx\int_0^\pi dy\int_0^\pi dz\ \frac{\cos lx\cos my\cos nz}{t-\cos x-\gamma\cos y-\gamma\cos z} \qquad (2.1)$$

Comparison of (2.1) with (1.2) shows that

$$G(t;l,m,n)=\frac{1}{\pi}\int_0^\pi dx\cos lx\ G(t-\cos x;m,n;\gamma,0) \qquad (2.2)$$

Thus we can obtain the value of the lattice Green's function for the tetragonal lattice at an arbitrary point for all the ranges of s by the numerical integration. Putting $\gamma=1$. we also obtain the value for the s.c. lattice.

3. B.C.C. Lattice

The lattice Green's function for the b.c.c. lattice is given by

$$G(t;l,m,n)=\frac{1}{\pi^3}\int_0^\pi dx\int_0^\pi dy\int_0^\pi dz\ \frac{\cos lx\cos my\cos nz}{t-\cos x\cos y\cos z} \tag{3.1}$$

Comparison of (3.1) with (1.2) shows that

$$G(t;l,m,n)=\frac{1}{\pi}\int_0^\pi dx\cos lx\ G(t;m,n;0,\cos x)\ . \tag{3.2}$$

Thus we can obtain the value of the lattice Green's function for the b.c.c. lattice. However the more convenient method for calculating the lattice Green's function for the b.c.c. lattice was studied by Morita.[10]

4. F.C.C. Lattice

The lattice Green's function for the f.c.c. lattice is given by

$$G(t;l,m,n)=\frac{1}{\pi^3}\int_0^\pi dx\int_0^\pi dy\int_0^\pi dz\ \frac{\cos lx\cos my\cos nz}{t-\cos x\cos y-\cos y\cos z-\cos z\cos x} \tag{4.1}$$

Comparison of (4.1) with (1.2) shows that

$$G(t;l,m,n)=\frac{1}{\pi}\int_0^\pi dx\ \cos lx\ G(t;m,n;\cos x,1) \tag{4.2}$$

This value is obtained by the numerical integration.

5. S.C. Lattice with the Nearest, the Next Nearest and the Third Nearest Neighbor Interactions

The lattice Green's function for the s.c. lattice with the nearest, the next nearest and the third nearest neighbor interactions is given by

$$G(t;l,m,n)$$

$$= \frac{1}{\pi^3}\int_0^\pi dx\int_0^\pi dy\int_0^\pi dz \; \frac{\cos lx \cos my \cos nz}{t-\alpha(\cos x+\cos y+\cos z)-\beta(\cos x\cos y+\cos y\cos z+\cos z\cos x)-\gamma\cos x\cos y\cos z} \tag{5.1}$$

Comparison of (5.1) with (1.2) shows that

$$G(t;l,m,n)=\frac{1}{\pi}\int_0^\pi dx \cos lx \; G(t-\alpha\cos x\,;m,n\,;\alpha+\beta\cos x,\beta+\gamma\cos x) \tag{5.2}$$

Thus we can obtain this value by a numerical integration.

6. B.C.C. Lattice with the Nearest and the Next Nearest Neighbor Interactions

The lattice Green's function for the square lattice with the nearest and the next nearest neighbor interactions is given by another form as follows:

$$G'(t;m,n) = \frac{1}{\pi^2}\int_0^\pi dy\int_0^\pi dz \; \frac{\cos my \cos nz}{t-2\gamma\cos y\cos z-\beta(\cos 2y+\cos 2z)}$$

$$= G\left(t;\frac{m+n}{2},\frac{m-n}{2};\gamma,2\beta\right) \tag{6.1}$$

On the other hand, the lattice Green's function for the b.c.c. lattice with the nearest and the next nearest neighbor interactions is given by

$$G(t;l,m,n)=\frac{1}{\pi^3}\int_0^\pi dx\int_0^\pi dy\int_0^\pi dz \; \frac{\cos lx\cos my\cos nz}{t-\alpha\cos x\cos y\cos z-\beta(\cos 2x+\cos 2y+\cos 2z)} \tag{6.2}$$

Comparison of (6.2) with (6.1) shows that

$$G(t;l,m,n)=\frac{1}{\pi}\int_0^{\pi}dx\cos lx\ G\left(t-\beta\cos 2x;\frac{m+n}{2},\frac{m-n}{2};\frac{\alpha}{2}\cos x,2\beta\right) \quad (6.3)$$

Thus we can obtain this value by a numerical integration.

7. Concluding Remarks

The formulas useful for the calculation of the lattice Green's functions at the arbitrary lattice point for the square lattice with the nearest and the next nearest neighbor interactions, the s.c., tetragonal, b.c.c.and f.c.c. lattices with the nearest neighbor interaction, the s.c. lattice with the nearest, the next nearest and the third nearest neighbor interactions and the b.c.c. lattice with the nearest and the next nearest neighbor interactions are drived for the whole range, $-\infty < s < \infty$. We confirm that these formulas provide the useful subroutines for the numerical calculations. Details will be reported in the near future.